

## Foreword

Traditional medicine has, since its inception, registered numerous examples of treatment resulting in positive or negative outcomes, depending on the patient. This observation was reinforced after the completion of the human genome sequencing project. As it turns out, individual humans exhibit genetic differences despite possessing the same genome. The identification of so-called single nucleotide polymorphisms confirms and explains the familiar phenomenon of variable reaction to treatment [1, 2]. Given that even siblings differ in terms of their chromosomal material, the genetic variability of the general human population should come as no surprise. Recent research has also revealed differences in the composition of gut bacterial flora resulting from diverse dietary habits [3]. In light of such specificities, the need for individual, personalized therapy becomes evident. Fortunately, many high-tech tools can be used in medical practice (Chapter 1).

The most direct applications of personalized medicine involve individualized pharmacotherapy. Drugs designed to interact with a specific target may help improve therapeutic outcomes while remaining affordable, particularly in the presence of bioinformatic technologies. Identifying links between molecular chemistry and pathological processes is among the goals of system biology [4]. Access to computer software that simulates the complete proteome may help discover causal reactions—not just in the scope of a particular disease, but between seemingly unconnected processes occurring in the organism [4]. Harnessing the power of modern computers in an objective, dispassionate therapeutic process will enhance the capabilities of medical practitioners, for example, by offering access to vast databases of biological and medical knowledge (Chapter 2). Moreover, processing data with the use of artificial intelligence algorithms may lead to conclusions which a human would not otherwise be able to reach (Chapter 2).

Closer collaboration between communication system experts and biologists should help identify promising research directions and explain the methods by which organisms—the most complex biological systems known to man—identify and process information (Chapter 3).

Gaining insight into the molecular phenomena will help resolve some long-standing fundamental questions. Even before this happens, however, medical science can reap benefits by exploiting existing solutions and models (Chapter 4).

Eliminating transplant rejection is of critical importance in individualized therapy. Three-dimensional bioprinting technologies represent an important milestone on this path (Chapter 5). They can be used to build arbitrarily complex objects, with local variations in the applied materials. An advanced printing environment may enable introduction of biological material (e.g., cells harvested from the patient for whom the implant is being created) directly at the printing stage (Chapter 5). Similarly, the shape of the printed tissue may accurately reflect the patient's needs, which

is particularly important, e.g., when recreating the layout of coronary vessels for bypass surgery.

Surgeons may also benefit greatly from the use of robots that surpass humans in their capacity to perform repetitive actions with great accuracy (Chapter 6).

Modern diagnostic tools that both simplify the therapeutic process and improve its accuracy already provide added value for doctors. A hybrid operating room that supports both macro- and microscale (cellular) activities enhances on-the-fly decision making during surgery (Chapter 7).

Recent advances in augmented reality technologies are finding their way into the operating theater, assisting surgeons and enabling them to make the right choices as the surgery progresses. Holographically superimposing imaging results (such as CAT scans) on the actual view of the patient's body (made possible by AR headsets) enhances the surgeon's precision and eliminates errors caused by inaccurate identification of the surgical target (Chapters 8 and 9).

The use of computers in medical research also encompasses the organization system of a hospital. The software monitoring information and transport of materials (as well as medical equipment) in hospital units delivers the logistic system for the communication of patients and doctors in medical practice (Chapter 10).

The medical treatment takes advantage of applying the techniques of telecommunication, allowing the conduct of therapy and especially surgery independently between medical doctors participating in the therapeutic practice from a distance (Chapter 11).

Medical education implements the training simulation using phantoms. The computer-based steering of phantom behavior allows the medical students to be familiar with the patient's behavior in extreme conditions, conscienceless, or rising emotions (Chapter 12).

This publication should be regarded as an extension of our previous work, presenting the use of simulation techniques in studying systems of variable structural complexity (including the human organism [5]). The overview presented simulations carried out at several scales, from individual molecules, through cells and organs, all the way to the organism as a whole.

The simulation of diagnostic processes is presented with the use of so-called virtual patients, whereas therapeutic approaches are discussed on the example of chemotherapy. We also present psychological aspects related to gamification and describe 3D printing as a means of treating skeletal defects. In this hierarchy of ever-greater involvement of IT technologies, the final tier is occupied by telemedicine. All tiers are discussed against the backdrop of preclinical activities described in the previous edition of *Simulations in Medicine*.

The current overview focuses on the use of simulation techniques in clinical practice and decision support, particularly in delivering personalized therapeutic solutions. Personalized therapy is currently the focus of significant research effort in areas such as genomics, epigenetics, drug design, and nutrition, while also yielding

practical benefits, such as those described in the presented work. The subject has engendered numerous publications, some of which are explicitly mentioned in our study.

Both editions of *Simulations in Medicine* demonstrate the extensive practical applications of *in silico* solutions. The marriage of medicine and information science promises to result in tools and approaches that facilitate large-scale adoption of personalized therapy. It seems, however, that the effective design of personalized treatment options calls for better understanding of processes such as protein folding and 3D structure prediction. Pathologies that affect the folding process lead to a variety of medical conditions jointly referred to as misfolding diseases. This phenomenon is among the most pressing challenges facing modern medical research [6–18].

## References

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